



RESEARCH CENTER
Bordeaux - Sud-Ouest

FIELD

Activity Report 2018

Section Application Domains

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AUCTUS Team

4. Application Domains

4.1. Factory 4.0

The 4th industrial revolution (factory 4.0) is characterized by the integration of digital technologies into the production process, in order to meet the challenge of customizing services and products. This agility requires making manufacturing and maintenance lines flexible and versatile. This capacity for adaptation is the characteristic of the human being, which puts him at the center of the production apparatus. However, this can no longer be done at the expense of their health and well-being. How then can we reconcile the enhancement of our manual and analytical expertise, the ever desired increase in productivity and manufacturing quality, while reducing the hardship at work? Collaborative robotics, which we are seeking to build, is one of the central solutions to meet this societal challenge. By assisting humans in their most dangerous and painful tasks, it complements or replaces them in their phases of physical and cognitive fragility.

More generally, we are interested in workstation cobotization, in the manufacturing and assembly industry but also in the construction and craft industries. The application areas are related to regional needs in aeronautics, including maintenance, water and waste treatment. In most of these cases, it is possible to define the tasks, evaluate the stakes and added value of our work.

CAGIRE Project-Team

4. Application Domains

4.1. Aeronautics

Cagire is presently involved in studies mainly related to:

- The combustion chamber wall: the modelling, the simulation and the experimentation of the flow around a multiperforated plate representative of a real combustion chamber wall are the three axes we have been developing during the recent period. The continuous improvement of our in-house test facility Maveric is also an important ingredient to produce our own experimental validation data for isothermal flows. For non-isothermal flows, our participation in the EU funded program Soprano will be giving us access to non-isothermal data produced by Onera.
- The flow around airfoils: the modelling of the turbulent boundary layer has been for almost a century a key issue in the aeronautics industry. However, even the more advanced RANS models face difficulties in predicting the influence of pressure gradients on the development of the boundary layer. A main issue is the reliability of the modelling hypotheses, which is crucial for less conservative design. One of the technological barriers is the prediction of the flow in regimes close to the edge of the flight domain (stall, buffeting, unsteady loads) when the boundary layer is slowed down by an adverse pressure gradient. This is the subject of the CIFRE PhD thesis of Gustave Sporschill, started in 2018, in collaboration with Dassault Aviation.

4.2. Power stations

R. Manceau has established a long term collaboration (4 CIFRE PhD theses in the past, 2 ongoing) with the R & D center of EDF of Chatou, for the development of refined turbulence models in the in-house CFD code of EDF, Code_Saturne :

- The prediction of heat transfer in fluid and solid components is of major importance in power stations, in particular, nuclear power plants. Either for the thermohydraulics of the plenum or in the study of accidental scenarii, among others, the accurate estimation of wall heat transfer, mean temperatures and temperature fluctuations are necessary for the evaluation of relevant thermal and mechanical design criteria. The PhD thesis (CIFRE EDF) of G. Mangeon is dedicated to the development of relevant RANS models for these industrial applications.
- Moreover, the prediction of unsteady hydrodynamic loadings is a key point for operating and for safety studies of PWR power plants. Currently, the static loading is correctly predicted by RANS computations but when the flow is transient (as, for instance, in Reactor Coolant Pumps, due to rotor/stator interactions, or during operating transients) or in the presence of large, energetic, coherent structures in the external flow region, the RANS approach is not sufficient, whereas LES is still too costly for a wide use in industry. This issue constitutes the starting point of the just-started PhD thesis (CIFRE EDF) of Vladimir Duffal.

4.3. Automotive propulsion

- The engine (underhood) compartment is a key component of vehicle design, in which the temperature is monitored to ensure the effectiveness and safety of the vehicle, and participates in 5 to 8% of the total drag and CO₂ emissions. Dimensioning is an aerodynamic and arothermal compromise, validated on a succession of road stages at constant speed and stopped phases (red lights, tolls, traffic jam). Although CFD is routinely used for forced convection, state-of-the-art turbulence models are not able to reproduce flows dominated by natural convection during stopped phases, with a Rayleigh

number of the order of 10^{10} , such that the design still relies on costly, full-scale, wind tunnel experiments. This technical barrier must be lifted, since the ambition of the PSA group is to reach a *full digital design of their vehicles in the 2025 horizon*, i.e., to almost entirely rely on CFD. This issue is the focus of the ongoing PhD thesis (CIFRE PSA) of S. Jameel, supervised by R. Manceau, and also a part of the ANR project MONACO_2025 described in section 9.2.2 .

- The Power & Vehicles Division of IFPEN co-develops a CFD code to simulate the internal flow in a spark-ignition engine, in order to provide the automotive industry with tools to optimize the design of combustion engines. The RANS method, widely used in the industry, is not sufficiently reliable for quantitative predictions, and is only used as a tool to qualitatively compare different geometries. On the other hand, LES provides more detailed and accurate information, but at the price of a CPU cost unaffordable for daily use in the industry. Therefore, IFPEN aims at developing the hybrid RANS/LES methodology, in order to combine the strengths of the two approaches. The PhD thesis of Hassan Afailal, co-supervised by Rémi Manceau, is focused on this issue.

CARDAMOM Project-Team

4. Application Domains

4.1. De-anti icing systems

Impact of large ice debris on downstream aerodynamic surfaces and ingestion by aft mounted engines must be considered during the aircraft certification process. It is typically the result of ice accumulation on unprotected surfaces, ice accretions downstream of ice protected areas, or ice growth on surfaces due to delayed activation of ice protection systems (IPS) or IPS failure. This raises the need for accurate ice trajectory simulation tools to support pre-design, design and certification phases while improving cost efficiency. Present ice trajectory simulation tools have limited capabilities due to the lack of appropriate experimental aerodynamic force and moment data for ice fragments and the large number of variables that can affect the trajectories of ice particles in the aircraft flow field like the shape, size, mass, initial velocity, shedding location, etc... There are generally two types of model used to track shed ice pieces. The first type of model makes the assumption that ice pieces do not significantly affect the flow. The second type of model intends to take into account ice pieces interacting with the flow. We are concerned with the second type of models, involving fully coupled time-accurate aerodynamic and flight mechanics simulations, and thus requiring the use of high efficiency adaptive tools, and possibly tools allowing to easily track moving objects in the flow. We will in particular pursue and enhance our initial work based on adaptive immersed boundary capturing of moving ice debris, whose movements are computed using basic mechanical laws.

In [51] it has been proposed to model ice shedding trajectories by an innovative paradigm that is based on Cartesian grids, PEnalization and LLevel Sets (LESCAPE code). Our objective is to use the potential of high order unstructured mesh adaptation and immersed boundary techniques to provide a geometrically flexible extension of this idea. These activities will be linked to the development of efficient mesh adaptation and time stepping techniques for time dependent flows, and their coupling with the immersed boundary methods we started developing in the FP7 EU project STORM [45], [100]. In these methods we compensate for the error at solid walls introduced by the penalization by using anisotropic mesh adaptation [73], [89], [90]. From the numerical point of view one of the major challenges is to guarantee efficiency and accuracy of the time stepping in presence of highly stretched adaptive and moving meshes. Semi-implicit, locally implicit, multi-level, and split discretizations will be explored to this end.

Besides the numerical aspects, we will deal with modelling challenges. One source of complexity is the initial conditions which are essential to compute ice shedding trajectories. It is thus extremely important to understand the mechanisms of ice release. With the development of next generations of engines and aircraft, there is a crucial need to better assess and predict icing aspects early in design phases and identify breakthrough technologies for ice protection systems compatible with future architectures. When a thermal ice protection system is activated, it melts a part of the ice in contact with the surface, creating a liquid water film and therefore lowering ability of the ice block to adhere to the surface. The aerodynamic forces are then able to detach the ice block from the surface [53]. In order to assess the performance of such a system, it is essential to understand the mechanisms by which the aerodynamic forces manage to detach the ice. The current state of the art in icing codes is an empirical criterion. However such an empirical criterion is unsatisfactory. Following the early work of [56], [50] we will develop appropriate asymptotic PDE approximations allowing to describe the ice formation and detachment, trying to embed in this description elements from damage/fracture mechanics. These models will constitute closures for aerodynamics/RANS and URANS simulations in the form of PDE wall models, or modified boundary conditions.

In addition to this, several sources of uncertainties are associated to the ice geometry, size, orientation and the shedding location. In very few papers [104], some sensitivity analysis based on Monte Carlo method have been conducted to take into account the uncertainties of the initial conditions and the chaotic nature of the ice particle motion. We aim to propose some systematic approach to handle every source of uncertainty in an efficient way relying on some state-of-art techniques developed in the Team. In particular, we will perform an uncertainty propagation of some uncertainties on the initial conditions (position, orientation, velocity,...) through a low-fidelity model in order to get statistics of a multitude of particle tracks. This study will be done in collaboration with ETS (Ecole de Technologies Supérieure, Canada). The longterm objective is to produce footprint maps and to analyse the sensitivity of the models developed.

4.2. Space re-entry

As already mentioned, atmospheric re-entry involves multi-scale fluid flow physics including highly rarefied effects, aerothermochemistry, radiation. All this must be coupled to the response of thermal protection materials to extreme conditions. This response is most often the actual objective of the study, to allow the certification of Thermal Protection Systems (TPS).

One of the applications we will consider is the so-called post-flight analysis of a space mission. This involves reconstructing the history of the re-entry module (trajectory and flow) from data measured on the spacecraft by means of a Flush Air Data System (FADS), a set of sensors flush mounted in the thermal protection system to measure the static pressure (pressure taps) and heat flux (calorimeters). This study involves the accurate determination of the freestream conditions during the trajectory. In practice this means determining temperature, pressure, and Mach number in front of the bow shock forming during re-entry. As shown by zur Nieden and Olivier [121], state of the art techniques for freestream characterization rely on several approximations, such as e.g. using an equivalent calorically perfect gas formulas instead of taking into account the complex aero-thermo-chemical behaviour of the fluid. These techniques do not integrate measurement errors nor the heat flux contribution, for which a correct knowledge drives more complex models such as gas surface interaction. In this context, CFD supplied with UQ tools permits to take into account chemical effects and to include both measurement errors and epistemic uncertainties, e.g. those due to the fluid approximation, on the chemical model parameters in the bulk and at the wall (surface catalysis).

Rebuilding the freestream conditions from the stagnation point data therefore amounts to solving a stochastic inverse problem, as in robust optimization. Our objective is to build a robust and global framework for rebuilding freestream conditions from stagnation-point measurements for the trajectory of a re-entry vehicle. To achieve this goal, methods should be developed for

- an accurate simulation of the flow in all the regimes, from rarefied, to transitional, to continuous ;
- providing a complete analysis about the reliability and the prediction of the numerical simulation in hypersonic flows, determining the most important source of error in the simulation (PDE model, discretization, mesh, etc)
- reducing the overall computational cost of the analysis .

Our work on the improvement of the simulation capabilities for re-entry flows will focus both on the models and on the methods. We will in particular provide an approach to extend the use of standard CFD models in the transitional regime, with CPU gains of several orders of magnitude w.r.t. Boltzmann solvers. To do this we will use the results of a boundary layer analysis allowing to correct the Navier-Stokes equations. This theory gives modified (or extended) boundary conditions that are called "slip velocity" and "temperature jump" conditions. This theory seems to be completely ignored by the aerospace engineering community. Instead, people rather use a simpler theory due to Maxwell that also gives slip and jump boundary conditions: however, the coefficients given by this theory are not correct. This is why several teams have tried to modify these coefficients by some empirical methods, but it seems that this does not give any satisfactory boundary conditions.

Our project is twofold. First, we want to revisit the asymptotic theory, and to make it known in the aerospace community. Second, we want to make an intensive sensitivity analysis of the model to the various coefficients of the boundary conditions. Indeed, there are two kinds of coefficients in these boundary conditions. The first one is the accommodation coefficient: in the kinetic model, it gives the proportion of molecules that are specularly reflected, while the others are reflected according to a normal distribution (the so-called diffuse reflexion). This coefficient is a data of the kinetic model that can be measured by experiments: it depends on the material and the structure of the solid boundary, and of the gas. Its influence on the results of a Navier-Stokes simulation is certainly quite important. The other coefficients are those of the slip and jump boundary conditions: they are issued from the boundary layer analysis, and we have absolutely no idea of the order of magnitude of their influence on the results of a Navier-Stokes solution. In particular, it is not clear if these results are more sensitive to the accommodation coefficient or to these slip and jump coefficients.

In this project, we shall make use of the expertise of the team on uncertainty quantification to investigate the sensitivity of the Navier-Stokes model with slip and jump coefficients to these various coefficients. This would be rather new in the field of aerospace community. It could also have some impacts in other sciences in which slip and jump boundary conditions with incorrect coefficients are still used, like for instance in spray simulations: for very small particles immersed in a gas, the drag coefficient is modified to account for rarefied effects (when the radius of the particle is of the same order of magnitude as the mean free path in the gas), and slip and jump boundary conditions are used.

Another application which has very close similarities to the physics of de-anti icing systems is the modelling of the solid and liquid ablation of the thermal protective system of the aircraft. This involves the degradation and recession of the solid boundary of the protection layer due to the heating generated by the friction. As in the case of de-anti icing systems, the simulation of these phenomena need to take into account the heat conduction in the solid, its phase change, and the coupling between a weakly compressible and a compressible phase. Fluid/Solid coupling methods are generally based on a weak approach. Here we will both study, by theoretical and numerical techniques, a strong coupling method for the interaction between the fluid and the solid, and, as for de-anti icing systems, attempt at developing appropriate asymptotic models. These would constitute some sort of thin layer/wall models to couple to the external flow solver.

These modelling capabilities will be coupled to high order adaptive discretizations to provide high fidelity flow models. One of the most challenging problems is the minimization of the influence of mesh and scheme on the wall conditions on the re-entry module. To reduce this influence, we will investigate both high order adaptation across the bow shock, and possibly adaptation based on uncertainty quantification high order moments related to the heat flux estimation, or shock fitting techniques [54], [95]. These tools will be coupled to our robust inverse techniques. One of our objectives is to development of a low-cost strategy for improving the numerical prediction by taking into account experimental data. Some methods have been recently introduced [103] for providing an estimation of the numerical errors/uncertainties. We will use some metamodels for solving the inverse problem, by considering all sources of uncertainty, including those on physical models. We will validate the framework using the experimental data available in strong collaboration with the von Karman Institute for Fluid dynamics (VKI). In particular, data coming from the VKI Longshot facility will be used. We will show application of the developed numerical tool for the prediction in flight conditions.

These activities will benefit from our strong collaborations with the CEA and with the von Karman Institute for Fluid Dynamics and ESA.

4.3. Energy

We will develop modelling and design tools, as well as dedicated platforms, for Rankine cycles using complex fluids (organic compounds), and for wave energy extraction systems.

Organic Rankine Cycles (ORCs) use heavy organic compounds as working fluids. This results in superior efficiency over steam Rankine cycles for source temperatures below 900 K. ORCs typically require only a single-stage rotating component making them much simpler than typical multi-stage steam turbines. The strong pressure reduction in the turbine may lead to supersonic flows in the rotor, and thus to the appearance of shocks, which reduces the efficiency due to the associated losses. To avoid this, either a larger multi stage installation is used, in which smaller pressure drops are obtained in each stage, or centripetal turbines are used, at very high rotation speeds (of the order of 25,000 rpm). The second solution allows to keep the simplicity of the expander, but leads to poor turbine efficiencies (60-80%) - w.r.t. modern, highly optimized, steam and gas turbines - and to higher mechanical constraints. The use of *dense-gas working fluids*, i.e. operating close to the saturation curve, in properly chosen conditions could increase the turbine critical Mach number avoiding the formation of shocks, and increasing the efficiency. Specific shape optimization may enhance these effects, possibly allowing the reduction of rotation speeds. However, dense gases may have significantly different properties with respect to dilute ones. Their dynamics is governed by a thermodynamic parameter known as the fundamental derivative of gas dynamics

$$\Gamma = 1 + \frac{\rho}{c} \left(\frac{\partial c}{\partial \rho} \right)_s, \quad (1)$$

where ρ is the density, c is the speed of sound and s is the entropy. For ideal gas $\Gamma = (\gamma + 1)/2 > 1$. For some complex fluids and some particular conditions of pressure and temperature, Γ may be lower than one, implying that $(\partial c / \partial \rho)_s < 0$. This means that the acceleration of pressure perturbations through a variable density fluids may be reversed and become a deceleration. It has been shown that, for $\Gamma \ll 1$, compression shocks are strongly reduced, thus alleviating the shock intensity. This has great potential in increasing the efficiency. This is why so much interest is put on dense gas ORCs.

The simulation of these gases requires accurate thermodynamic models, such as Span-Wagner or Peng-Robinson (see [66]). The data to build these models is scarce due to the difficulty of performing reliable experiments. The related uncertainty is thus very high. Our work will go in the following directions:

1. develop deterministic models for the turbine and the other elements of the cycle. These will involve multi-dimensional high fidelity, as well as intermediate and low fidelity (one- and zero-dimensional), models for the turbine, and some 0D/1D models for other element of the cycle (pump, condenser, etc) ;
2. validation of the coupling between the various elements. The following aspects will be considered: characterization of the uncertainties on the cycle components (e.g. empirical coefficients modelling the pump or the condenser), calibration of the thermodynamic parameters, model the uncertainty of each element, and the influence of the unsteady experimental data ;
3. demonstrate the interest of a specific optimization of geometry, operating conditions, and the choice of the fluid, according to the geographical location by including local solar radiation data. Multi-objective optimization will be considered to maximize performance indexes (e.g. Carnot efficiency, mechanical work and energy production), and to reduce the variability of the output.

This work will provide modern tools for the robust design of ORCs systems. It benefits from the direct collaboration with the SME EXOES (ANR LabCom VIPER), and from a collaboration with LEMMA.

Wave energy conversion is an emerging sector in energy engineering. The design of new and efficient Wave Energy Converters (WECs) is thus a crucial activity. As pointed out by Weber [120], it is more economical to raise the technology performance level (TPL) of a wave energy converter concept at low technology readiness level (TRL). Such a development path puts a greater demand on the numerical methods used. The findings of Weber also tell us that important design decisions as well as optimization should be performed as early in the development process as possible. However, as already mentioned, today the wave energy sector relies heavily on the use of tools based on simplified linear hydrodynamic models for the prediction of motions, loads, and power production. Our objective is to provide this sector, and especially SMEs, with robust design tools to minimize the uncertainties in predicted power production, loads, and costs of wave energy.

Following our initial work [76], we will develop, analyse, compare, and use for multi-fidelity optimization, non-linear models of different scales (fidelity) ranging from simple linear hydrodynamics over asymptotic discrete nonlinear wave models, to non-hydrostatic anisotropic Euler free surface solvers. We will not work on the development of small scale models (VOF-RANS or LES) but may use such models, developed by our collaborators, for validation purposes. These developments will benefit from all our methodological work on asymptotic modelling and high order discretizations. As shown in [76], asymptotic models for WECs involve an equation for the pressure on the body inducing a PDE structure similar to that of incompressible flow equations. The study of appropriate stable and efficient high order approximations (coupling velocity-pressure, efficient time stepping) will be an important part of this activity. Moreover, the flow-floating body interaction formulation introduces time stepping issues similar to those encountered in fluid structure interaction problems, and require a clever handling of complex floater geometries based on adaptive and ALE techniques. For this application, the derivation of fully discrete asymptotics may actually simplify our task.

Once available, we will use this hierarchy of models to investigate and identify the modelling errors, and provide a more certain estimate of the cost of wave energy. Subsequently we will look into optimization cycles by comparing time-to-decision in a multi-fidelity optimization context. In particular, this task will include the development and implementation of appropriate surrogate models to reduce the computational cost of expensive high fidelity models. Here especially artificial neural networks (ANN) and Kriging response surfaces (KRS) will be investigated. This activity on asymptotic non-linear modelling for WECs, which has had very little attention in the past, will provide entirely new tools for this application. Multi-fidelity robust optimization is also an approach which has never been applied to WECs.

This work is the core of the EU OCEANERanet MIDWEST project, which we coordinate. It will be performed in collaboration with our European partners, and with a close supervision of European SMEs in the sector, which are part of the steering board of MIDWEST (WaveDragon, Waves4Power, Tecnalia).

4.4. Materials engineering

Because of their high strength and low weight, ceramic-matrix composite materials (CMCs) are the focus of active research for aerospace and energy applications involving high temperatures, either military or civil. Though based on brittle ceramic components, these composites are not brittle due to the use of a fibre/matrix interphase that preserves the fibres from cracks appearing in the matrix. Recent developments aim at implementing also in civil aero engines a specific class of Ceramic Matrix Composite materials (CMCs) that show a self-healing behaviour. Self-healing consists in filling cracks appearing in the material with a dense fluid formed in-situ by oxidation of part of the matrix components. Self-healing (SH) CMCs are composed of a complex three-dimensional topology of woven fabrics containing fibre bundles immersed in a matrix coating of different phases. The oxide seal protects the fibres which are sensitive to oxidation, thus delaying failure. The obtained lifetimes reach hundreds of thousands of hours [108].

The behaviour of a fibre bundle is actually extremely variable, as the oxidation reactions generating the self-healing mechanism have kinetics strongly dependent on temperature and composition. In particular, the lifetime of SH-CMCs depends on: (i) temperature and composition of the surrounding atmosphere; (ii) composition and topology of the matrix layers; (iii) the competition of the multidimensional diffusion/oxidation/volatilization processes; (iv) the multidimensional flow of the oxide in the crack; (v) the inner topology of fibre bundles; (vi) the distribution of critical defects in the fibres. Unfortunately, experimental investigations on the full materials are too long (they can last years) and their output too qualitative (the coupled effects can only be observed a-posteriori on a broken sample). Modelling is thus essential to study and to design SH-CMCs.

In collaboration with the LCTS laboratory (a joint CNRS-CEA-SAFRAN-Bordeaux University lab devoted to the study of thermo-structural materials in Bordeaux), we are developing a multi-scale model in which a structural mechanics solver is coupled with a closure model for the crack physico chemistry. This model is obtained as a multi-dimensional asymptotic crack averaged approximation for the transport equations (Fick's laws) with chemical reactions sources, plus a potential model for the flow of oxide [69], [74], [105]. We

have demonstrated the potential of this model in showing the importance of taking into account the multi-dimensional topology of a fibre bundle (distribution of fibres) in the rupture mechanism. This means that the 0-dimensional model used in most of the studies (see e.g. [64]) will underestimate appreciably the lifetime of the material. Based on these recent advances, we will further pursue the development of multi-scale multi-dimensional asymptotic closure models for the parametric design of self healing CMCs. Our objectives are to provide: (i) new, non-linear multi-dimensional mathematical model of CMCs, in which the physico-chemistry of the self-healing process is more strongly coupled to the two-phase (liquid gas) hydro-dynamics of the healing oxide ; (ii) a model to represent and couple crack networks ; (iii) a robust and efficient coupling with the structural mechanics code ; (iv) validate this platform with experimental data obtained at the LCTS laboratory. The final objective is to set up a multi-scale platform for the robust prediction of lifetime of SH-CMCs, which will be a helpful tool for the tailoring of the next generation of these materials.

4.5. Coastal and civil engineering

Our objective is to bridge the gap between the development of high order adaptive methods, which has mainly been performed in the industrial context and environmental applications, with particular attention to coastal and hydraulic engineering. We want to provide tools for adaptive non-linear modelling at large and intermediate scales (near shore, estuarine and river hydrodynamics). We will develop multi-scale adaptive models for free surface hydrodynamics. Beside the models and codes themselves, based on the most advanced numerics we will develop during this project, we want to provide sufficient know how to control, adapt and optimize these tools.

We will focus our effort in the understanding of the interactions between asymptotic approximations and numerical approximations. This is extremely important in at least two aspects. The first is the capability of a numerical model to handle highly dispersive wave propagation. This is usually done by high accuracy asymptotic PDE expansions. Here we plan to make heavily use of our results concerning the relations between vertical asymptotic expansions and standard finite element approximations. In particular, we will invest some effort in the development of $xy+z$ adaptive finite element approximations of the incompressible Euler equations. Local p -adaptation of the vertical approximation may provide a “variable depth” approximation exploiting numerics instead of analytical asymptotics to control the physical behaviour of the model.

Another important aspect which is not understood well enough at the moment is the role of dissipation in wave breaking regions. There are several examples of breaking closure, going from algebraic and PDE-based eddy viscosity methods [86], [110], [102], [71], to hybrid methods coupling dispersive PDEs with hyperbolic ones, and trying to mimic wave breaking with travelling bores [114], [115], [113], [84], [77]. In both cases, numerical dissipation plays an important role and the activation or not of the breaking closure, as the quantitative contribution of numerical dissipation to the flow has not been properly investigated. These elements must be clarified to allow full control of adaptive techniques for the models used in this type of applications.

Another point we want to clarify is how to optimize the discretization of asymptotic PDE models. In particular, when adding mesh size(s) and time step, we are in presence of at least 3 (or even more) small parameters. The relations between physical ones have been more or less investigated, as have been the ones between purely numerical ones. We plan to study the impact of numerics on asymptotic PDE modelling by reverting the usual process and studying asymptotic limits of finite element discretizations of the Euler equations. Preliminary results show that this does allow to provide some understanding of this interaction and to possibly propose considerably improved numerical methods [52].

CARMEN Project-Team

4. Application Domains

4.1. Scientific context: the LIRYC

The University Hospital of Bordeaux (*CHU de Bordeaux*) is equipped with a specialized cardiology hospital, the *Hôpital Cardiologique du Haut-Lévêque*, where the group of Professor Michel Haïssaguerre has established itself as a global leader in the field of cardiac electrophysiology [58], [57], [47]. Their discoveries in the area of atrial fibrillation and sudden cardiac death syndromes are widely acclaimed, and the group is a national and international referral center for treatment of cardiac arrhythmia. Thus the group also sees large numbers of patients with rare cardiac diseases.

In 2011 the group has won the competition for a 40 million euro *Investissements d'Avenir* grant for the establishment of IHU Liryc, an institute that combines clinical, experimental, and numerical research in the area of cardiac arrhythmia (<http://ihu-liryc.fr>). The institute works in all areas of modern cardiac electrophysiology: atrial arrhythmias, sudden death due to ventricular fibrillation, heart failure related to ventricular dyssynchrony, and metabolic disorders. It is recognized as one of the most important centers worldwide in this area.

The Carmen team was founded to partner with IHU Liryc. We bring applied mathematics and scientific computing closer to experimental and clinical cardiac electrophysiology. In collaboration with experimental and clinical researchers at Liry we work to enhance fundamental knowledge of the normal and abnormal cardiac electrical activity and of the patterns of the electrocardiogram, and we develop new simulation tools for training, biological, and clinical applications.

4.2. Basic experimental electrophysiology

Our modeling is carried out in coordination with the experimental teams from IHU Liryc. It help to write new concepts concerning the multiscale organisation of the cardiac action potentials that will serve our understanding in many electrical pathologies. For example, we model the structural heterogeneities at the cellular scale [31], and at an intermediate scale between the cellular and tissue scales.

At the atrial level, we apply our models to understand the mechanisms of complex arrhythmias and the relation with the heterogeneities at the insertion of the pulmonary veins. We will model the heterogeneities specific to the atria, like fibrosis or fatty infiltration [34] [56]. These heterogeneities ara thought to play a major role in the development of atrial fibrillation.

At the ventricular level, we focus on (1) modeling the complex coupling between the Purkinje network and the ventricles, which is supposed to play a major role in sudden cardiac death, and (2) modeling the heteogeneities related to the complex organization and disorganization of the myocytes and fibroblasts, which is important in the study of infarct scars for instance.

4.3. Clinical electrophysiology

Treatment of cardiac arrhythmia is possible by pharmacological means, by implantation of pacemakers and defibrillators, and by curative ablation of diseased tissue by local heating or freezing. In particular the ablative therapies create challenges that can be addressed by numerical means. Cardiologists would like to know, preferably by noninvasive means, where an arrhythmia originates and by what mechanism it is sustained.

We address this issue in the first place using inverse models, which attempt to estimate the cardiac activity from a (high-density) electrocardiogram. A new project aims at performing this estimation on-site in the catheterization laboratory and presenting the results, together with the cardiac anatomy, on the screen that the cardiologist uses to monitor the catheter positions [40].

An important prerequisite for this kind of interventions and for inverse modeling is the creation of anatomical models from imaging data. The Carmen team contributes to better and more efficient segmentation and meshing through the IDAM project.

CQFD Project-Team

4. Application Domains

4.1. Dependability and safety

Our abilities in probability and statistics apply naturally to industry, in particular in studies of dependability and safety. An illustrative example is the collaboration that started in September 2014 with THALES Optronique. The goal of this project is the optimization of the maintenance of an onboard system equipped with a HUMS (Health Unit Monitoring Systems). The physical system under consideration is modeled by a piecewise deterministic Markov process. In the context of impulse control, we propose a dynamic maintenance policy, adapted to the state of the system and taking into account both random failures and those related to the degradation phenomenon.

The spectrum of applications of the topics that the team can address is large and can concern many other fields. Indeed non parametric and semi-parametric regression methods can be used in biometry, econometrics or engineering for instance. Gene selection from microarray data and text categorization are two typical application domains of dimension reduction among others. We had for instance the opportunity via the scientific program PRIMEQUAL to work on air quality data and to use dimension reduction techniques as principal component analysis (PCA) or positive matrix factorization (PMF) for pollution sources identification and quantization.

FLOWERS Project-Team

4. Application Domains

4.1. Application Domains

Neuroscience, Developmental Psychology and Cognitive Sciences The computational modelling of life-long learning and development mechanisms achieved in the team centrally targets to contribute to our understanding of the processes of sensorimotor, cognitive and social development in humans. In particular, it provides a methodological basis to analyze the dynamics of the interaction across learning and inference processes, embodiment and the social environment, allowing to formalize precise hypotheses and later on test them in experimental paradigms with animals and humans. A paradigmatic example of this activity is the Neurocuriosity project achieved in collaboration with the cognitive neuroscience lab of Jacqueline Gottlieb, where theoretical models of the mechanisms of information seeking, active learning and spontaneous exploration have been developed in coordination with experimental evidence and investigation, see <https://flowers.inria.fr/neurocuriosityproject/>.

Personal and lifelong learning robotics Many indicators show that the arrival of personal robots in homes and everyday life will be a major fact of the 21st century. These robots will range from purely entertainment or educative applications to social companions that many argue will be of crucial help in our society. Yet, to realize this vision, important obstacles need to be overcome: these robots will have to evolve in unpredictable homes and learn new skills in a lifelong manner while interacting with non-engineer humans after they left factories, which is out of reach of current technology. In this context, the refoundation of intelligent systems that developmental robotics is exploring opens potentially novel horizons to solve these problems. In particular, this application domain requires advances in artificial intelligence that go beyond the current state-of-the-art in fields like deep learning. Currently these techniques require tremendous amounts of data in order to function properly, and they are severely limited in terms of incremental and transfer learning. One of our goals is to drastically reduce the amount of data required in order for this very potent field to work. We try to achieve this by making neural networks aware of their knowledge, i.e. we introduce the concept of uncertainty, and use it as part of intrinsically motivated multitask learning architectures, and combined with techniques of learning by imitation.

Human-Robot Collaboration. Robots play a vital role for industry and ensure the efficient and competitive production of a wide range of goods. They replace humans in many tasks which otherwise would be too difficult, too dangerous, or too expensive to perform. However, the new needs and desires of the society call for manufacturing system centered around personalized products and small series productions. Human-robot collaboration could widen the use of robot in this new situations if robots become cheaper, easier to program and safe to interact with. The most relevant systems for such applications would follow an expert worker and works with (some) autonomy, but being always under supervision of the human and acts based on its task models.

Environment perception in intelligent vehicles. When working in simulated traffic environments, elements of FLOWERS research can be applied to the autonomous acquisition of increasingly abstract representations of both traffic objects and traffic scenes. In particular, the object classes of vehicles and pedestrians are of interest when considering detection tasks in safety systems, as well as scene categories ("scene context") that have a strong impact on the occurrence of these object classes. As already indicated by several investigations in the field, results from present-day simulation technology can be transferred to the real world with little impact on performance. Therefore, applications of FLOWERS research that is suitably verified by real-world benchmarks has direct applicability in safety-system products for intelligent vehicles.

Automated Tutoring Systems. Optimal teaching and efficient teaching/learning environments can be applied to aid teaching in schools aiming both at increase the achievement levels and the reduce time needed. From a practical perspective, improved models could be saving millions of hours of students' time (and effort) in learning. These models should also predict the achievement levels of students in order to influence teaching practices.

GEOSTAT Project-Team

4. Application Domains

4.1. Sparse signals & optimisation

This research topic involves **Geostat** team and is used to set up an InnovationLab with **I2S company**

Sparsity can be used in many ways and there exist various sparse models in the literature; for instance minimizing the l_0 quasi-norm is known to be an NP-hard problem as one needs to try all the possible combinations of the signal's elements. The l_1 norm, which is the convex relaxation of the l_0 quasi-norm results in a tractable optimization problem. The l_p pseudo-norms with $0 < p < 1$ are particularly interesting as they give closer approximation of l_0 but result in a non-convex minimization problem. Thus, finding a global minimum for this kind of problem is not guaranteed. However, using a non-convex penalty instead of the l_1 norm has been shown to improve significantly various sparsity-based applications. Nonconvexity has a lot of statistical implications in signal and image processing. Indeed, natural images tend to have a heavy-tailed (kurtotic) distribution in certain domains such as wavelets and gradients. Using the l_1 norm comes to consider a Laplacian distribution. More generally, the hyper-Laplacian distribution is related to the l_p pseudo-norm ($0 < p < 1$) where the value of p controls how the distribution is heavy-tailed. As the hyper-Laplacian distribution for $0 < p < 1$ represents better the empirical distribution of the transformed images, it makes sense to use the l_p pseudo-norms instead of l_1 . Other functions that better reflect heavy-tailed distributions of images have been used as well such as Student-t or Gaussian Scale Mixtures. The internal properties of natural images have helped researchers to push the sparsity principle further and develop highly efficient algorithms for restoration, representation and coding. Group sparsity is an extension of the sparsity principle where data is clustered into groups and each group is sparsified differently. More specifically, in many cases, it makes sense to follow a certain structure when sparsifying by forcing similar sets of points to be zeros or non-zeros simultaneously. This is typically true for natural images that represent coherent structures. The concept of group sparsity has been first used for simultaneously shrinking groups of wavelet coefficients because of the relations between wavelet basis elements. Lastly, there is a strong relationship between sparsity, nonpredictability and scale invariance.

We have shown that the two powerful concepts of sparsity and scale invariance can be exploited to design fast and efficient imaging algorithms. A general framework has been set up for using non-convex sparsity by applying a first-order approximation. When using a proximal solver to estimate a solution of a sparsity-based optimization problem, sparse terms are always separated in subproblems that take the form of a proximal operator. Estimating the proximal operator associated to a non-convex term is thus the key component to use efficient solvers for non-convex sparse optimization. Using this strategy, only the shrinkage operator changes and thus the solver has the same complexity for both the convex and non-convex cases. While few previous works have also proposed to use non-convex sparsity, their choice of the sparse penalty is rather limited to functions like the l_p pseudo-norm for certain values of $p \geq 0.5$ or the Minimax Concave (MC) penalty because they admit an analytical solution. Using a first-order approximation only requires calculating the (super)gradient of the function, which makes it possible to use a wide range of penalties for sparse regularization. This is important in various applications where we need a flexible shrinkage function such as in edge-aware processing. Apart from non-convexity, using a first-order approximation makes it easier to verify the optimality condition of proximal operator-based solvers via fixed-point interpretation. Another problem that arises in various imaging applications but has attracted less works is the problem of multi-sparsity, when the minimization problem includes various sparse terms that can be non-convex. This is typically the case when looking for a sparse solution in a certain domain while rejecting outliers in the data-fitting term. By using one intermediate variable per sparse term, we show that proximal-based solvers can be efficient. We give a detailed study of the Alternating Direction Method of Multipliers (ADMM) solver for multi-sparsity and study its properties. The following subjects are addressed and receive new solutions:

- **Edge aware smoothing:** given an input image g , one seeks a smooth image u "close" to g by minimizing:

$$\operatorname{argmin}_u \frac{\lambda}{2} \|u - g\|_2^2 + \psi(\nabla u)$$

where ψ is a sparsity-inducing non-convex function and λ a positive parameter. Splitting and alternate minimization lead to the sub-problems:

$$\begin{aligned} \text{(sp1)} & : v^{(k+1)} \leftarrow \operatorname{argmin}_v \psi(v) + \frac{\beta}{2} \|\nabla u^{(k)} - v\|_2^2 \\ \text{(sp2)} & : u^{(k+1)} \leftarrow \operatorname{argmin}_u \lambda \|u - g\|_2^2 + \beta \|\nabla u - v^{(k+1)}\|_2^2. \end{aligned}$$

We solve sub-problem (sp2) through deconvolution and efficient estimation via separable filters and warm-start initialization for fast GPU implementation, and sub-problem (sp1) through non-convex proximal form.

- **Structure-texture separation:** design of an efficient algorithm using non-convex terms on both the data-fitting and the prior. The resulting problem is solved via a combination of Half-Quadratic (HQ) and Maximization-Minimization (MM) methods. We extract challenging texture layers outperforming existing techniques while maintaining a low computational cost. Using spectral sparsity in the framework of low-rank estimation, we propose to use robust Principal Component Analysis (RPCA) to perform robust separation on multi-channel images such as glare and artifacts removal of flash/no-flash photographs. As in this case, the matrix to decompose has much less columns than lines, we propose to use a QR decomposition trick instead of a direct singular value decomposition (SVD) which makes the decomposition faster.

- **Robust integration:** in many applications, we need to reconstruct an image from corrupted gradient fields. The corruption can take the form of outliers only when the vector field is the result of transformed gradient fields (low-level vision), or mixed outliers and noise when the field is estimated from corrupted measurements (surface reconstruction, gradient camera, Magnetic Resonance Imaging (MRI) compressed sensing, etc.). We use non-convexity and multi-sparsity to build efficient integrability enforcement algorithms. We present two algorithms : 1) a local algorithm that uses sparsity in the gradient field as a prior together with a sparse data-fitting term, 2) a non-local algorithm that uses sparsity in the spectral domain of non-local patches as a prior together with a sparse data-fitting term. Both methods make use of a multi-sparse version of the Half-Quadratic solver. The proposed methods were the first in the literature to propose a sparse regularization to improve integration. Results produced with these methods significantly outperform previous works that use no regularization or simple l_1 minimization. Exact or near-exact recovery of surfaces is possible with the proposed methods from highly corrupted gradient fields with outliers.

- **Learning image denoising:** deep convolutional networks that consist in extracting features by repeated convolutions with high-pass filters and pooling/downsampling operators have shown to give near-human recognition rates. Training the filters of a multi-layer network is costly and requires powerful machines. However, visualizing the first layers of the filters shows that they resemble wavelet filters, leading to sparse representations in each layer. We propose to use the concept of scale invariance of multifractals to extract invariant features on each sparse representation. We build a bi-Lipschitz invariant descriptor based on the distribution of the singularities of the sparsified images in each layer. Combining the descriptors of each layer in one feature vector leads to a compact representation of a texture image that is invariant to various transformations. Using this descriptor that is efficient to calculate with learning techniques such as classifiers combination and artificially adding training data, we build a powerful texture recognition system that outperforms previous works on 3 challenging datasets. In fact, this system leads to quite close recognition rates compared to latest advanced deep nets while not requiring any filters training.

HIEPACS Project-Team

4. Application Domains

4.1. Material physics

Participants: Olivier Coulaud, Pierre Esterie, Arnaud Durocher, Oguz Kaya.

Due to the increase of available computer power, new applications in nano science and physics appear such as study of properties of new materials (photovoltaic materials, bio- and environmental sensors, ...), failure in materials, nano-indentation. Chemists, physicists now commonly perform simulations in these fields. These computations simulate systems up to billion of atoms in materials, for large time scales up to several nanoseconds. The larger the simulation, the smaller the computational cost of the potential driving the phenomena, resulting in low precision results. So, if we need to increase the precision, there are two ways to decrease the computational cost. In the first approach, we improve algorithms and their parallelization and in the second way, we will consider a multiscale approach.

A domain of interest is the material aging for the nuclear industry. The materials are exposed to complex conditions due to the combination of thermo-mechanical loading, the effects of irradiation and the harsh operating environment. This operating regime makes experimentation extremely difficult and we must rely on multi-physics and multi-scale modeling for our understanding of how these materials behave in service. This fundamental understanding helps not only to ensure the longevity of existing nuclear reactors, but also to guide the development of new materials for 4th generation reactor programs and dedicated fusion reactors. For the study of crystalline materials, an important tool is dislocation dynamics (DD) modeling. This multiscale simulation method predicts the plastic response of a material from the underlying physics of dislocation motion. DD serves as a crucial link between the scale of molecular dynamics and macroscopic methods based on finite elements; it can be used to accurately describe the interactions of a small handful of dislocations, or equally well to investigate the global behavior of a massive collection of interacting defects.

To explore i.e. to simulate these new areas, we need to develop and/or to improve significantly models, schemes and solvers used in the classical codes. In the project, we want to accelerate algorithms arising in those fields. We will focus on the following topics (in particular in the currently under definition **OPTIDIS** project in collaboration with CEA Saclay, CEA Ile-de-france and SIMaP Laboratory in Grenoble) in connection with research described at Sections 3.4 and 3.5 .

- The interaction between dislocations is long ranged ($O(1/r)$) and anisotropic, leading to severe computational challenges for large-scale simulations. In dislocation codes, the computation of interaction forces between dislocations is still the most CPU time consuming and has to be improved to obtain faster and more accurate simulations.
- In such simulations, the number of dislocations grows while the phenomenon occurs and these dislocations are not uniformly distributed in the domain. This means that strategies to dynamically construct a good load balancing are crucial to achieve high performance.
- From a physical and a simulation point of view, it will be interesting to couple a molecular dynamics model (atomistic model) with a dislocation one (mesoscale model). In such three-dimensional coupling, the main difficulties are firstly to find and characterize a dislocation in the atomistic region, secondly to understand how we can transmit with consistency the information between the two micro and meso scales.

4.2. Co-design for scalable numerical algorithms in scientific applications

Participants: Emmanuel Agullo, Nicolas Bouzat, Mathieu Faverge, Luc Giraud, Matthieu Kuhn, Gilles Marait, Louis Poirel, Pierre Ramet, Jean Roman.

4.2.1. High performance simulation for ITER tokamak

Scientific simulation for ITER tokamak modeling provides a natural bridge between theory and experimentation and is also an essential tool for understanding and predicting plasma behavior. Recent progresses in numerical simulation of fine-scale turbulence and in large-scale dynamics of magnetically confined plasma have been enabled by access to petascale supercomputers. These progresses would have been unreachable without new computational methods and adapted reduced models. In particular, the plasma science community has developed codes for which computer runtime scales quite well with the number of processors up to thousands cores. The research activities of HIEPACS concerning the international ITER challenge were involved in the Inria Project Lab C2S@Exa in collaboration with CEA-IRFM and are related to two complementary studies: a first one concerning the turbulence of plasma particles inside a tokamak (in the context of GYSELA code) and a second one concerning the MHD instability edge localized modes (in the context of JOREK code).

Currently, GYSELA is parallelized in an hybrid MPI+OpenMP way and can exploit the power of the current greatest supercomputers. To simulate faithfully the plasma physic, GYSELA handles a huge amount of data and today, the memory consumption is a bottleneck on very large simulations. In this context, mastering the memory consumption of the code becomes critical to consolidate its scalability and to enable the implementation of new numerical and physical features to fully benefit from the extreme scale architectures.

Other numerical simulation tools designed for the ITER challenge aim at making a significant progress in understanding active control methods of plasma edge MHD instability Edge Localized Modes (ELMs) which represent a particular danger with respect to heat and particle loads for Plasma Facing Components (PFC) in the tokamak. The goal is to improve the understanding of the related physics and to propose possible new strategies to improve effectiveness of ELM control techniques. The simulation tool used (JOREK code) is related to non linear MHD modeling and is based on a fully implicit time evolution scheme that leads to 3D large very badly conditioned sparse linear systems to be solved at every time step. In this context, the use of PaStiX library to solve efficiently these large sparse problems by a direct method is a challenging issue.

4.2.2. Numerical and parallel scalable hybrid solvers in large scale calculations

Parallel and numerically scalable hybrid solvers based on a fully algebraic coarse space correction have been theoretically studied and various advanced parallel implementations have been designed. Their parallel scalability has been investigated on large scale problems within the EoCoE project thanks to a close collaboration with the BSC and the integration of MaPHYs within the Alya software. The performance has also been assessed on PRACE Tier-0 machine within a PRACE Project Access through a collaboration with CERFACS and Laboratoire de Physique des Plasmas at École Polytechnique for the calculation of plasma propulsion.

LFANT Project-Team (section vide)

MAGIQUE-3D Project-Team

4. Application Domains

4.1. Seismic Imaging

The main objective of modern seismic processing is to find the best representation of the subsurface that can fit the data recorded during the seismic acquisition survey. In this context, the seismic wave equation is the most appropriate mathematical model. Numerous research programs and related publications have been devoted to this equation. An acoustic representation is suitable if the waves propagate in a fluid. But the subsurface does not contain fluids only and the acoustic representation is not sufficient in the general case. Indeed the acoustic wave equation does not take some waves into account, for instance shear waves, turning waves or the multiples that are generated after several reflections at the interfaces between the different layers of the geological model. It is then necessary to consider a mathematical model that is more complex and resolution techniques that can model such waves. The elastic or viscoelastic wave equations are then reference models, but they are much more difficult to solve, in particular in the 3D case. Hence, we need to develop new high-performance approximation methods.

Reflection seismics is an indirect measurement technique that consists in recording echoes produced by the propagation of a seismic wave in a geological model. This wave is created artificially during seismic acquisition surveys. These echoes (i.e., reflections) are generated by the heterogeneities of the model. For instance, if the seismic wave propagates from a clay layer to sand, one will observe a sharp reflected signal in the seismic data recorded in the field. One then talks about reflection seismics if the wave is reflected at the interface between the two media, or talks about seismic refraction if the wave is transmitted along the interface. The arrival time of the echo enables one to locate the position of this transition, and the amplitude of the echo gives information on some physical parameters of the two geological media that are in contact. The first petroleum exploration surveys were performed at the beginning of the 1920's and for instance, the Orchard Salt Dome in Texas (USA) was discovered in 1924 by the seismic-reflection method.

4.2. Imaging complex media with ultrasonic waves

The acoustic behavior of heterogeneous or composite materials attracts considerable excitement. Indeed, their acoustic response may be extremely different from the single constituents responses. In particular, dispersions of resonators in a matrix are the object of large research efforts, both experimentally and theoretically. However it is still a challenge to dispose of numerical tools with sufficient abilities to deal with the simulation and imaging of such materials behavior. Indeed, not only acoustic simulations are very time-consuming, but they have to be performed on realistic enough solution domains, i.e. domains which capture well enough the structural features of the considered materials.

This collaboration with I2M, University of Bordeaux aims at addressing this type of challenges by developing numerical and experimental tools in order to understand the propagation of ultrasonic waves in complex media, image these media, and in the future, help design composite materials for industrial purposes.

4.3. Helioseismology

This collaboration with the Max Planck Institute for Solar System, Göttingen, Germany, which started in 2014, aims at designing efficient numerical methods for the wave propagation problems that arise in helioseismology in the context of inverse problems. The final goal is to retrieve information about the structure of the Sun i.e. inner properties such as density or pressure via the inversion of a wave propagation problem. Acoustic waves propagate inside the Sun which, in a first approximation and regarding the time scales of physical phenomena, can be considered as a moving fluid medium with constant velocity of motion. Some other simplifications lead to computational saving, such as supposing a radial or axisymmetric geometry of the Sun.

Aeroacoustic equations must be adapted and efficiently solved in this context, this has been done in the finite elements code Montjoie. In other situations, a full 3D simulation is required and demands large computational resources. Ultimately, we aim at modeling the coupling with gravity potential and electromagnetic waves (MHD equations) in order to be able to better understand Sun spots.

MANAO Project-Team

4. Application Domains

4.1. Physical Systems

Given our close relationships with researchers in optics, one novelty of our approach is to extend the range of possible observers to physical sensors in order to work on domains such as simulation, mixed reality, and testing. Capturing, processing, and visualizing complex data is now more and more accessible to everyone, leading to the possible convergence of real and virtual worlds through visual signals. This signal is traditionally captured by cameras. It is now possible to augment them by projecting (e.g., the infrared laser of Microsoft Kinect) and capturing (e.g., GPS localization) other signals that are outside the visible range. This supplemental information replaces values traditionally extracted from standard images and thus lowers down requirements in computational power. Since the captured images are the result of the interactions between light, shape, and matter, the approaches and the improved knowledge from *MANAO* help in designing interactive acquisition and rendering technologies that are required to merge the real and the virtual worlds. With the resulting unified systems (optical and digital), transfer of pertinent information is favored and inefficient conversion is likely avoided, leading to new uses in interactive computer graphics applications, like **augmented reality**, **displays** and **computational photography**.

4.2. Interactive Visualization and Modeling

This direction includes domains such as **scientific illustration and visualization**, **artistic or plausible rendering**, and **3D modeling**. In all these cases, the observer, a human, takes part in the process, justifying once more our focus on real-time methods. When targeting average users, characteristics as well as limitations of the human visual system should be taken into account: in particular, it is known that some configurations of light, shape, and matter have masking and facilitation effects on visual perception. For specialized applications (such as archeology), the expertise of the final user and the constraints for 3D user interfaces lead to new uses and dedicated solutions for models and algorithms.

MEMPHIS Project-Team

4. Application Domains

4.1. Energy conversion

We apply the methods developed in our team to the domain of wind engineering and sea-wave converters. In Figure 1, we show results of a numerical model for a sea-wave energy converter. We here rely on a monolithic model to describe the interaction between the rigid floater, air and water; material properties such as densities, viscosities and rigidity vary across the domain. The appropriate boundary conditions are imposed at interfaces that arbitrarily cross the grid using adapted schemes built thanks to geometrical information computed via level set functions [43]. The background method for fluid-structure interface is the volume penalization method [25] where the level set functions is used to improve the degree of accuracy of the method [3] and also to follow the object. The underlined mathematical model is unsteady, and three dimensional; numerical simulations based on a grid with $\mathcal{O}(10^8)$ degrees of freedom are executed in parallel using 512 CPUs .

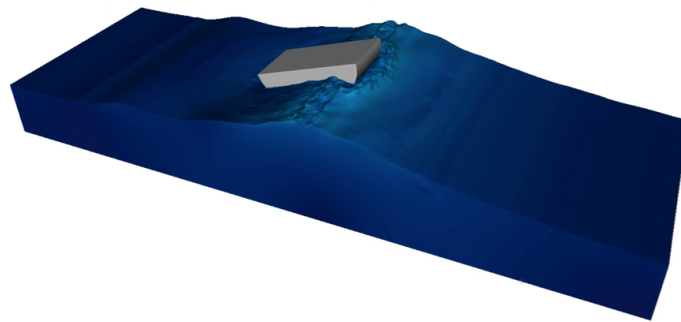


Figure 1. numerical modeling of a sea-wave converter by a monolithic model and Cartesian meshes.

In the context of the Aerogust (Aeroelastic gust modelling) European project, together with Valorem, we investigated the behavior of wind turbine blades under gust loading. The aim of the project was to optimize the design of wind turbine blades to maximize the power extracted. A meteorological mast (Figure 2 (a)) has been installed in Brittany in March 2017 to measure wind on-site: data provided by the mast have been exploited to initialize the mathematical model. Due to the large cost of the full-order mathematical model, we relied on a simplified model [35] to optimize the global twist. Then, we validated the optimal configuration using the full-order Cartesian model based on the NaSCar solver. Figure 2 (b) shows the flow around the optimized optimized wind turbine rotor.

4.2. Impacts

Mathematical and numerical modelling of physical systems undergoing impacts is challenging due to the presence of large deformations and displacements of the solid part, and due to the strongly non-linear behaviour of the fluid part. At the same time, proper experiments of impact phenomena are particularly dangerous and require expensive facilities, which make them largely impractical. For this reason, there is a growing interest in the development of predictive models for impact phenomena.



Figure 2. Aerogust project. Left: met mast after its installation. Right: flow around the optimized wind turbine rotor (as predicted by NaSCar).

In MEMPHIS, we rely on a fully Eulerian approach based on conservation laws, where the different materials are characterized by their specific constitutive laws, to address these tasks. This approach was introduced in [34] and subsequently pursued and extended in [40], [33], [27], [30]. In Figure 3, we show the results of the numerical simulation of the impact of a copper projectile immersed in air over a copper shield. Results are obtained using a fully parallel monolithic Cartesian method, based on a 4000^2 fixed Cartesian grid. Simulations are performed on a cluster of 512 processors, and benefits from the isomorphism between grid partitioning and processor topology.

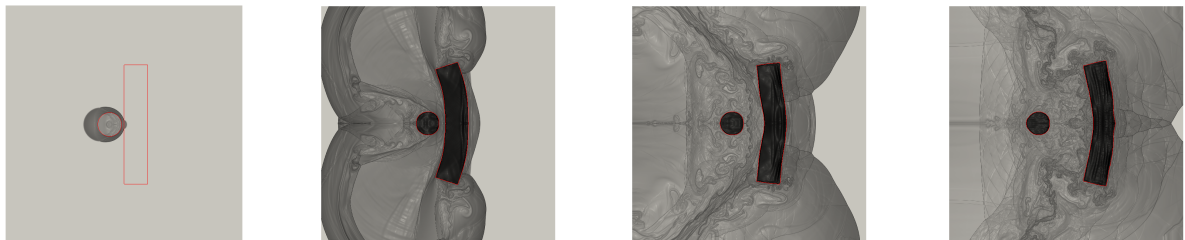


Figure 3. impact and rebound of a copper projectile on a copper plate. Interface and schlieren at $50\mu s$, $199\mu s$, $398\mu s$ and $710\mu s$.

4.3. Vascular flows

A new research direction pursued by the team is the mathematical modelling of vascular blood flows in arteries. Together with the start-up Nurea (<http://nurea-soft.com/>) and the surgeon Eric Ducasse, we aim at developing reliable and automatic procedures for aneurysm segmentation and for the prediction of aneurysm rupture risk. Our approach exploits two sources of information: (i) numerical simulations of blood flows in complex geometries, based on an octree discretization, and (ii) computed tomography angiography (CTA) data. Figure

4 shows the force distribution on the walls of the abdominal aorta in presence of an aneurysm; results are obtained using a parallelized hierarchical Cartesian scheme based on octrees.

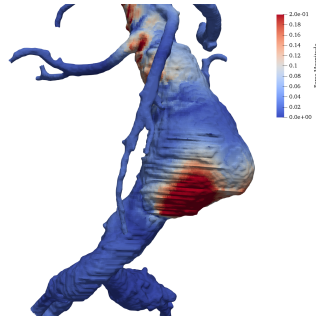


Figure 4. force distribution on the walls of the abdominal aorta in presence of an aneurysm.

MNEMOSYNE Project-Team

4. Application Domains

4.1. Overview

One of the most original specificity of our team is that it is part of a laboratory in Neuroscience (with a large spectrum of activity from the molecule to the behavior), focused on neurodegenerative diseases and consequently working in tight collaboration with the medical domain. As a consequence, neuroscientists and the medical world are considered as the primary end-users of our researches. Beyond data and signal analysis where our expertise in machine learning may be possibly useful, our interactions are mainly centered on the exploitation of our models. They will be classically regarded as a way to validate biological assumptions and to generate new hypotheses to be investigated in the living. Our macroscopic models and their implementation in autonomous robots will allow an analysis at the behavioral level and will propose a systemic framework, the interpretation of which will meet aetiological analysis in the medical domain and interpretation of intelligent behavior in cognitive neuroscience.

The study of neurodegenerative diseases is targeted because they match the phenomena we model. Particularly, the Parkinson disease results from the death of dopaminergic cells in the basal ganglia, one of the main systems that we are modeling. The Alzheimer disease also results from the loss of neurons, in several cortical and extracortical regions. The variety of these regions, together with large mnesic and cognitive deficits, require a systemic view of the cerebral architecture and associated functions, very consistent with our approach.

Of course, numerical sciences are also impacted by our researches, at several levels. At a global level, we will propose new control architectures aimed at providing a higher degree of autonomy to robots, as well as machine learning algorithms working in more realistic environment. More specifically, our focus on some cognitive functions in closed loop with a real environment will address currently open problems. This is obviously the case for planning and decision making; this is particularly the case for the domain of affective computing, since motivational characteristics arising from the design of an artificial physiology allow to consider not only cold rational cognition but also hot emotional cognition. The association of both kinds of cognition is undoubtedly an innovative way to create more realistic intelligent systems but also to elaborate more natural interfaces between these systems and human users.

At last, we think that our activities in well-founded distributed computations and high performance computing are not just intended to help us design large scale systems. We also think that we are working here at the core of informatics and, accordingly, that we could transfer some fundamental results in this domain.

MONC Project-Team

4. Application Domains

4.1. Tumor growth monitoring and therapeutic evaluation

Each type of cancer is different and requires an adequate model. More specifically, we are currently working on the following diseases:

- Glioma (brain tumors) of various grades,
- Metastases to the lung, liver and brain from various organs,
- Soft-tissue sarcoma,
- Kidney cancer and its metastases,
- EGFR-mutated lung cancer.

In this context our application domains are:

- Image-driven patient-specific simulations of tumor growth and treatments,
- Parameter estimation and data assimilation of medical images.

4.2. Biophysical therapies

- Modeling of electrochemotherapy on biological and clinical scales,
- Evaluation of radiotherapy and radiofrequency ablation.

4.3. Experimental research in oncology

We use mathematical modeling as a tool to assist biological cancer research in testing mechanistic hypotheses and pharmacological research. More specifically, our applications include:

- Theoretical biology of the metastatic process: dynamics of a population of tumors in mutual interactions, dormancy, pre-metastatic and metastatic niche, quantification of metastatic potential and differential effects of anti-angiogenic therapies on primary tumor and metastases,
- Rational and personalized dosing and scheduling of anti-cancer drugs in monotherapy or in combination,
- Mathematical modeling of intra-tumor drug transport to optimize the design of nanoparticles

PHOENIX-POST Team

4. Application Domains

4.1. Assistive computing in the home

Participants: Rafik Belloum, Audrey Landuran, Stéphanie Giraud, Flora Gallet, Amandine Desrozier, Charles Consel, Bernard Serpette, Eugène Volanschi.

In this avenue of research, we have been developing a systemic approach to introducing an assisted living platform for the home of older adults. To do so, we formed an interdisciplinary team that allows (1) to identify the user needs from a gerontological and psychological viewpoint; (2) to propose assistive applications designed by human factors and HCI experts, in collaboration with caregivers and users; (3) to develop and test applications designed and developed by software engineers; (4) to conduct a field study to assess the benefits of the platform and assistive applications, in collaboration with caregivers, by deploying the system at the actual homes.

Our research activities for assistive computing in the home are conducted under the *HomeAssist* project. This work takes the form of a platform offering an online catalog of assistive applications that orchestrate an open-ended set of networked objects. Our platform leverages DiaSuite to quickly and safely develop applications at a high level.

Our scientific achievements include the design principles of our platform, its key features to effectively assist individuals in their home, field studies to validate HomeAssist, the expansion of HomeAssist to serve individuals with ID, and the technology transfer of HomeAssist. Note that a complete presentation of this work, from a Cognitive Science perspective, is given in the doctoral thesis of Lucile Dupuy published recently (2016).

4.1.1. Project-team positioning

There is a range of platforms for assisted living aimed at older adults that have been developed for more than a decade. Most of these platforms are used in a setting where participants come to a research apartment to perform certain tasks. This setting makes it difficult to assess user acceptance and satisfaction of the proposed approaches because the user does not interact with the technology on a daily basis, over a period of time. Furthermore, older adults adopt routines to optimize their daily functioning at home. This situation calls for field studies in a naturalistic setting to strengthen the evaluation of assisted living platforms.

HomeAssist innovates in that it supports independent living across the activities of daily living and is validated by field studies in naturalistic setting.

4.2. Assistive computing on-the-go

Participants: Cécile Mazon, Benjamin Hate, Hélène Sauzéon, Charles Consel.

We conduct research on assistive computing supported by mobile devices such as smart phones and tablets. Both research projects presented in this section are supported by tablets and leverage their functionalities to guide users with cognitive challenges performing activities and tasks, whether in mainstream schools to support inclusion or in residential settings to support their autonomy. The mobile nature of tablets allows to envision such devices as supporting users with cognitive challenges across a range of environments.

Many research projects bring cognitive-support applications to users based on tablets and smartphones. However, few projects equip users with such devices in actual mainstream environments, including stakeholders in the design process and targeting an autonomous usage of assistive applications. An additional originality of our approach is our interdisciplinary approach that allows us to integrate key psychological dimensions in our design, such as self-determination.

4.3. Life Plan

Participants: Audrey Landuran, Bernard N’Kaoua.

Elaboration of life plan is a major stage in the developmental trajectory of people with intellectual deficiency and is based on several capabilities : make choices, express them, be aware of their consequences, etc. However, these various capabilities can raise problems for people with Down syndrome. The aim of this project has been to design and validate a digital assistant that allows to help the individuals to make choices, to plan for the future and to define their life plan. The user centered methodology employed has allowed to involve the people with Down syndrome, their families and their caregivers in all stages of design. Different validations achieved attest for the accessible, friendly, funny character of the assistant and its ability to promote the expression of the life plan in accordance with individuals’ choices, wishes and desires.

The digital assistant is now available online at : <http://www.monprojetdevie.trisomie21-france.org/>.



Figure 2. Sample screenshots from the Life Plan website.

PLEIADE Team

4. Application Domains

4.1. Genome and transcriptome annotation, to model function

Sequencing genomes and transcriptomes provides a picture of how a biological system can function, or does function under a given physiological condition. Simultaneous sequencing of a group of related organisms is now a routine procedure in biological laboratories for studying a behavior of interest, and provides a marvelous opportunity for building a comprehensive knowledge base of the relations between genomes. Key elements in mining these relations are: classifying the genes in related organisms and the reactions in their metabolic networks, recognizing the patterns that describe shared features, and highlighting specific differences.

PLEIADE will develop applications in comparative genomics of related organisms, using new mathematical tools for representing compactly, at different scales of difference, comparisons between related genomes. New methods based on computational geometry refine these comparisons. Compact representations can be stored, exchanged, and combined. They will form the basis of new simultaneous genome annotation methods, linked directly to abductive inference methods for building functional models of the organisms and their communities.

Our ambition in biotechnology is to permit the design of synthetic or genetically selected organisms at an abstract level, and guide the modification or assembly of a new genome. Our effort is focused on two main applications: genetic engineering and synthetic biology of oil-producing organisms (biofuels in CAER, palm oils), and improving and selecting starter microorganisms used in winemaking (collaboration with the ISVV and the BioLaffort company).

4.1.1. Oil Palm lipid synthesis

The largest source of vegetable oil⁰ is the fruit mesocarp of the oil palm *Elaeis guineensis*, a remarkable tissue that can accumulate up to 90% oil, the highest level observed in the plant kingdom. The market share of oil palm is expected to increase in order to meet increased demand for vegetable oil, predicted to double by 2030 [18], be it as food or as a source of biofuels in Africa. A significant proportion of palm oil is produced on small estates that do not have access to efficient milling facilities, and run a great risk of spoilage through oil acidification. Improving palm oil quality through genetics and selection will result in economic gains [24] by addressing several targets such as improvement of oil yield, tuning of oil quality through the rate of unsaturated fatty acids or impairment of degradation processes. Furthermore, as genome biodiversity resides mostly in Africa, oil from African oil palms can vary greatly in fatty acid composition according to cultivar genetic differences and to weather conditions, and the precise mechanisms regulating this variability are not yet understood.

A growing body of molecular resources for studying oil palm fruit are making it possible to study and improve the quality and quantity of oil produced by oil palms. In particular, these oils can vary greatly in fatty acid composition, and while the precise mechanisms regulating this variability are not completely understood, establishing a link between oil palm genotype and phenotype appears increasingly feasible. PLEIADE will work with the CNRS/UB UMR 5200 (LBM), a laboratory with an established reputation in studying fatty acid metabolism in *E. guineensis*, to improve understanding of the links between genetic diversity and oil production, and participate in developing applications.

4.1.2. Engineering pico-algae

⁰32% of the world market share [24]

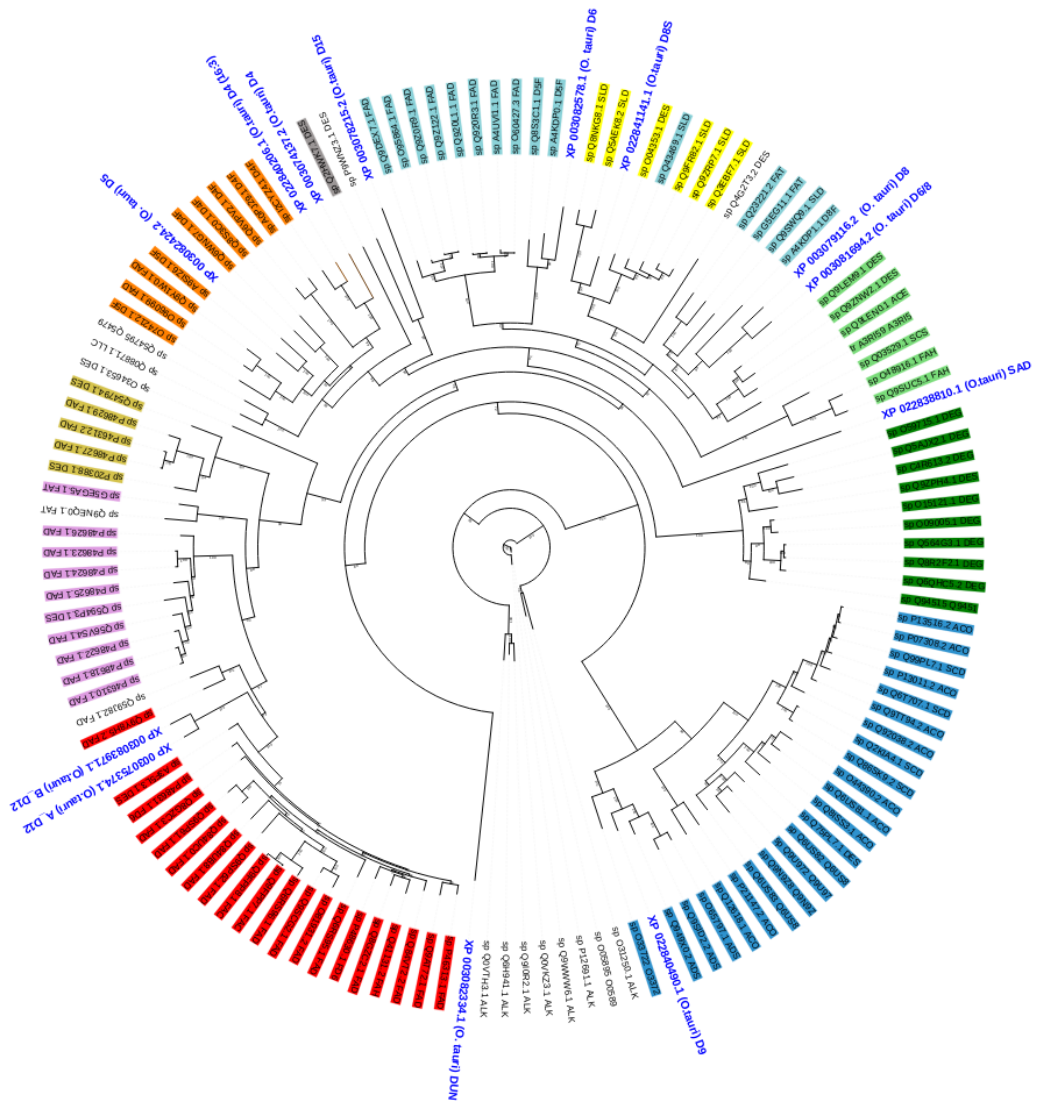


Figure 3. Phylogenetic structure of long-chain polyunsaturated fatty acid desaturase specificity. Highlighted are thirteen desaturases from *Ostreococcus tauri*

Docosahexaenoic acid (DHA) is an essential nutriment for human brain tissue and can only be obtained from marine or riverine fish that live on phytoplankton and zooplankton, since human neurons lack the delta desaturase required for *de novo* synthesis of DHA. [21] Unfortunately, fishing is become less and less a sustainable resource. Since phytoplankton and zooplankton are the ultimate source of DHA consumed, there is considerable interest in obtaining DHA directly rather than through the intermediary of fish. A very promising approach is through the bio-engineering of pico-algae.

In order to produce the long-chain polyunsaturated fatty acids (LC-PUFA) needed for human nutrition, it is necessary to precisely engineer the desaturases that produce them. Desaturases are enzymes responsible for the introduction of double bonds into fatty acids. Desaturases are specific in recognizing their substrates and in placing the double bond in the proper place. The desaturases that produce the LC-PUFA necessary for human nutrition are present only in some species.

Our goal is to design methods to predict the substrate and region specificities for desaturases in algal species, particularly *Ostreococcus tauri*, the smallest photosynthetic eukaryote that can be cultivated. Thirteen desaturases are known in *O. tauri* and can be placed in the phylogeny of the desaturase family (figure 3). The biochemical and structural characterization of these enzymes is as yet very incomplete. This work is ongoing (see section 8.2.3) and requires close collaboration between biologists and computer scientists.

4.2. Molecular based systematics and taxonomy

Defining and recognizing myriads of species in biosphere has taken phenomenal energy over the past centuries and remains a major goal of Natural History. It is an iconic paradigm in pattern recognition (clustering has coevolved with numerical taxonomy many decades ago). Developments in evolution and molecular biology, as well as in data analysis, have over the past decades enabled a profound revolution, where species can be delimited and recognized by data analysis of sequences. We aim at proposing new tools, in the framework of E-science, which make possible (i) better exploration of the diversity in a given clade, and (ii) assignment of a place in these patterns for new, unknown organisms, using information provided by sets of sequences. This will require investment in data analysis, machine learning, and pattern recognition to deal with the volumes of data and their complexity.

One example of this project is about the diversity of trees in Amazonian forest, in collaboration with botanists in French Guiana. Protists (unicellular Eukaryotes) are by far more diverse than plants, and far less known. Molecular exploration of Eukaryotes diversity is nowadays a standard in biodiversity studies. Data are available, through metagenomics, as an avalanche and make molecular diversity enter the domain of Big Data. Hence, an effort will be invested, in collaboration with other Inria teams (GenScale, HiePACS) for porting to HPC algorithms of pattern recognition and machine learning, or distance geometry, for these tools to be available as well in metagenomics. This will be developed first on diatoms (unicellular algae) in collaboration with INRA team at Thonon and University of Uppsala), on pathogens of tomato and grapewine, within an existing network, and on bacterial communities, in collaboration with University of Pau. For the latter, the studies will extend to correlations between molecular diversity and sets of traits and functions in the ecosystem.

4.3. Community ecology and population genetics

Community assembly models how species can assemble or disassemble to build stable or metastable communities. It has grown out of inventories of countable organisms. Using *metagenomics* one can produce molecular based inventories at rates never reached before. Most communities can be understood as pathways of carbon exchange, mostly in the form of sugar, between species. Even a plant cannot exist without carbon exchange with its rhizosphere. Two main routes for carbon exchange have been recognized: predation and parasitism. In predation, interactions—even if sometimes dramatic—may be loose and infrequent, whereas parasitism requires what Claude Combes has called intimate and sustainable interactions [19]. About one decade ago, some works [25] have proposed a comprehensive framework to link the studies of biodiversity with community assembly. This is still incipient research, connecting community ecology and biogeography.

We aim at developing graph-based models of co-occurrence between species from NGS inventories in metagenomics, i.e. recognition of patterns in community assembly, and as a further layer to study links, if any, between diversity at different scales and community assemblies, starting from current, but oversimplified theories, where species assemble from a regional pool either randomly, as in neutral models, or by environmental filtering, as in niche modeling. We propose to study community assembly as a multiscale process between nested pools, both in tree communities in Amazonia, and diatom communities in freshwaters. This will be a step towards community genomics, which adds an ecological flavour to metagenomics.

Convergence between the processes that shape genetic diversity and community diversity—drift, selection, mutation/speciation and migration—has been noted for decades and is now a paradigm, establishing a continuous scale between levels of diversity patterns, beyond classical approaches based on iconic levels like species and populations. We will aim at deciphering diversity pattern along these gradients, connecting population and community genetics. Therefore, some key points must be addressed on reliability of tools.

Next-generation sequencing technologies are now an essential tool in population and community genomics, either for making evolutionary inferences or for developing SNPs for population genotyping analyses. Two problems are highlighted in the literature related to the use of those technologies for population genomics: variable sequence coverage and higher sequencing error in comparison to the Sanger sequencing technology. Methods are developed to develop unbiased estimates of key parameters, especially integrating sequencing errors [23]. An additional problem can be created when sequences are mapped on a reference sequence, either the sequenced species or an heterologous one, since paralogous genes are then considered to be the same physical position, creating a false signal of diversity [20]. Several approaches were proposed to correct for paralogy, either by working directly on the sequences issued from mapped reads [20] or by filtering detected SNPs. Finally, an increasingly popular method (RADseq) is used to develop SNP markers, but it was shown that using RADseq data to estimate diversity directly biases estimates [12]. Workflows to implement statistical methods that correct for diversity biases estimates now need an implementation for biologists.

POTIOC Project-Team

4. Application Domains

4.1. Education

Education is at the core of the motivations of the Potioc group. Indeed, we are convinced that the approaches we investigate—which target motivation, curiosity, pleasure of use and high level of interactivity—may serve education purposes. To this end, we collaborate with experts in Educational Sciences and teachers for exploring new interactive systems that enhance learning processes. We are currently investigating the fields of astronomy, optics, and neurosciences. We are also working with special education centres for the blind on accessible augmented reality prototypes. In the future, we will continue exploring new interactive approaches dedicated to education, in various fields. Popularization of Science is also a key domain for Potioc. Focusing on this subject allows us to get inspiration for the development of new interactive approaches.

4.2. Art

Art, which is strongly linked with emotions and user experiences, is also a target area for Potioc. We believe that the work conducted in Potioc may be beneficial for creation from the artist point of view, and it may open new interactive experiences from the audience point of view. As an example, we are working with colleagues who are specialists in digital music, and with musicians. We are also working with jugglers and mockup builders with the goal of enhancing interactivity and user experience.

4.3. Entertainment

Similarly, entertainment is a domain where our work may have an impact. We notably explored BCI-based gaming and non-medical applications of BCI, as well as mobile Augmented Reality games. Once again, we believe that our approaches that merge the physical and the virtual world may enhance the user experience. Exploring such a domain will raise numerous scientific and technological questions.

4.4. Well-being

Finally, well-being is a domain where the work of Potioc can have an impact. We have notably shown that spatial augmented reality and tangible interaction may favor mindfulness activities, which have been shown to be beneficial for well-being. More generally, we explore *introspectibles* objects, which are tangible and augmented objects that are connected to physiological signals and that foster introspection. We explore these directions for general public, including people with special needs.

REALOPT Project-Team

4. Application Domains

4.1. Network Design and Routing Problems

We are actively working on problems arising in network topology design, implementing a survivability condition of the form “at least two paths link each pair of terminals”. We have extended polyhedral approaches to problem variants with bounded length requirements and re-routing restrictions [46]. Associated to network design is the question of traffic routing in the network: one needs to check that the network capacity suffices to carry the demand for traffic. The assignment of traffic also implies the installation of specific hardware at transient or terminal nodes.

To accommodate the increase of traffic in telecommunication networks, today’s optical networks use grooming and wavelength division multiplexing technologies. Packing multiple requests together in the same optical stream requires to convert the signal in the electrical domain at each aggregation of disaggregation of traffic at an origin, a destination or a bifurcation node. Traffic grooming and routing decisions along with wavelength assignments must be optimized to reduce opto-electronics system installation cost. We developed and compared several decomposition approaches [73], [71], [70] to deal with backbone optical network with relatively few nodes (around 20) but thousands of requests for which traditional multi-commodity network flow approaches are completely overwhelmed. We also studied the impact of imposing a restriction on the number of optical hops in any request route [69]. We also developed a branch-and-cut approach to a problem that consists in placing sensors on the links of a network for a minimum cost [51], [52].

The Dial-a-Ride Problem is a variant of the pickup and delivery problem with time windows, where the user inconvenience must be taken into account. In [62], ride time and customer waiting time are modeled through both constraints and an associated penalty in the objective function. We develop a column generation approach, dynamically generating feasible vehicle routes. Handling ride time constraints explicitly in the pricing problem solver requires specific developments. Our dynamic programming approach for pricing problem makes use of a heuristic dominance rule and a heuristic enumeration procedure, which in turns implies that our overall branch-and-price procedure is a heuristic. However, in practice our heuristic solutions are experimentally very close to exact solutions and our approach is numerically competitive in terms of computation times.

In [60], [59], we consider the problem of covering an urban area with sectors under additional constraints. We adapt the aggregation method to our column generation algorithm and focus on the problem of disaggregating the dual solution returned by the aggregated master problem.

We studied several time dependent formulations for the unit demand vehicle routing problem [36], [35]. We gave new bounding flow inequalities for a single commodity flow formulation of the problem. We described their impact by projecting them on some other sets of variables, such as variables issued of the Picard and Queyranne formulation or the natural set of design variables. Some inequalities obtained by projection are facet defining for the polytope associated with the problem. We are now running more numerical experiments in order to validate in practice the efficiency of our theoretical results.

We also worked on the p-median problem, applying the matching theory to develop an efficient algorithm in Y-free graphs and to provide a simple polyhedral characterization of the problem and therefore a simple linear formulation [68] simplifying results from Baiou and Barahona.

We considered the multi-commodity transportation problem. Applications of this problem arise in, for example, rail freight service design, “less than truckload” trucking, where goods should be delivered between different locations in a transportation network using various kinds of vehicles of large capacity. A particularity here is that, to be profitable, transportation of goods should be consolidated. This means that goods are not delivered directly from the origin to the destination, but transferred from one vehicle to another in intermediate locations. We proposed an original Mixed Integer Programming formulation for this problem which is suitable for resolution by a Branch-and-Price algorithm and intelligent primal heuristics based on it.

For the problem of routing freight railcars, we proposed two algorithms based on the column generation approach. These algorithms have been tested on a set of real-life instances coming from a real Russian freight transportation company. Our algorithms have been faster on these instances than the current solution approach being used by the company.

4.2. Packing and Covering Problems

Realopt team has a strong experience on exact methods for cutting and packing problems. These problems occur in logistics (loading trucks), industry (wood or steel cutting), computer science (parallel processor scheduling).

We developed a branch-and-price algorithm for the Bin Packing Problem with Conflicts which improves on other approaches available in the literature [67]. The algorithm uses our methodological advances like the generic branching rule for the branch-and-price and the column based heuristic. One of the ingredients which contributes to the success of our method are fast algorithms we developed for solving the subproblem which is the Knapsack Problem with Conflicts. Two variants of the subproblem have been considered: with interval and arbitrary conflict graphs.

We also developed a branch-and-price algorithm for a variant of the bin-packing problem where the items are fragile. In [24] we studied empirically different branching schemes and different algorithms for solving the subproblems.

We studied a variant of the knapsack problem encountered in inventory routing problem [54]: we faced a multiple-class integer knapsack problem with setups [53] (items are partitioned into classes whose use implies a setup cost and associated capacity consumption). We showed the extent to which classical results for the knapsack problem can be generalized to this variant with setups and we developed a specialized branch-and-bound algorithm.

We studied the orthogonal knapsack problem, with the help of graph theory [48], [47], [50], [49]. Fekete and Schepers proposed to model multi-dimensional orthogonal placement problems by using an efficient representation of all geometrically symmetric solutions by a so called *packing class* involving one *interval graph* for each dimension. Though Fekete & Schepers' framework is very efficient, we have however identified several weaknesses in their algorithms: the most obvious one is that they do not take advantage of the different possibilities to represent interval graphs. We propose to represent these graphs by matrices with consecutive ones on each row. We proposed a branch-and-bound algorithm for the 2D knapsack problem that uses our 2D packing feasibility check. We are currently developing exact optimization tools for glass-cutting problems in a collaboration with Saint-Gobain [29]. This 2D-3stage-Guillotine cut problems are very hard to solve given the scale of the instance we have to deal with. Moreover one has to issue cutting patterns that avoid the defaults that are present in the glass sheet that are used as raw material. There are extra sequencing constraints regarding the production that make the problem even more complex.

We have also organized a European challenge on packing with society Renault: see <https://paginas.fe.up.pt/~esicup/extern/esicup-12thMeeting/pmwiki.php?n=Conference.Info>. This challenge is about loading trucks under practical constraints.

4.3. Planning, Scheduling, and Logistic Problems

Inventory routing problems combine the optimization of product deliveries (or pickups) with inventory control at customer sites. We considered an industrial application where one must construct the planning of single product pickups over time; each site accumulates stock at a deterministic rate; the stock is emptied on each visit. We have developed a branch-and-price algorithm where periodic plans are generated for vehicles by solving a multiple choice knapsack subproblem, and the global planning of customer visits is coordinated by the master program [55]. We previously developed approximate solutions to a related problem combining vehicle routing and planning over a fixed time horizon (solving instances involving up to 6000 pick-ups and deliveries to plan over a twenty day time horizon with specific requirements on the frequency of visits to customers [57]).

Together with our partner company GAPSO from the associate team SAMBA, we worked on the equipment routing task scheduling problem [61] arising during port operations. In this problem, a set of tasks needs to be performed using equipments of different types with the objective to maximize the weighted sum of performed tasks.

We participated to the project on an airborne radar scheduling. For this problem, we developed fast heuristics [45] and exact algorithms [26]. A substantial research has been done on machine scheduling problems. A new compact MIP formulation was proposed for a large class of these problems [25]. An exact decomposition algorithm was developed for the NP-hard maximizing the weighted number of late jobs problem on a single machine [63]. A dominant class of schedules for malleable parallel jobs was discovered in the NP-hard problem to minimize the total weighted completion time [65]. We proved that a special case of the scheduling problem at cross docking terminals to minimize the storage cost is polynomially solvable [66], [64].

Another application area in which we have successfully developed MIP approaches is in the area of tactical production and supply chain planning. In [23], we proposed a simple heuristic for challenging multi-echelon problems that makes effective use of a standard MIP solver. [22] contains a detailed investigation of what makes solving the MIP formulations of such problems challenging; it provides a survey of the known methods for strengthening formulations for these applications, and it also pinpoints the specific substructure that seems to cause the bottleneck in solving these models. Finally, the results of [30] provide demonstrably stronger formulations for some problem classes than any previously proposed. We are now working on planning phytosanitary treatments in vineries.

We have been developing robust optimization models and methods to deal with a number of applications like the above in which uncertainty is involved. In [41], [40], we analyzed fundamental MIP models that incorporate uncertainty and we have exploited the structure of the stochastic formulation of the problems in order to derive algorithms and strong formulations for these and related problems. These results appear to be the first of their kind for structured stochastic MIP models. In addition, we have engaged in successful research to apply concepts such as these to health care logistics [31]. We considered train timetabling problems and their re-optimization after a perturbation in the network [43], [42]. The question of formulation is central. Models of the literature are not satisfactory: continuous time formulations have poor quality due to the presence of discrete decision (re-sequencing or re-routing); arc flow in time-space graph blow-up in size (they can only handle a single line timetabling problem). We have developed a discrete time formulation that strikes a compromise between these two previous models. Based on various time and network aggregation strategies, we develop a 2-stage approach, solving the contiguous time model having fixed the precedence based on a solution to the discrete time model.

Currently, we are conducting investigations on a real-world planning problem in the domain of energy production, in the context of a collaboration with EDF [37], [38], [39]. The problem consists in scheduling maintenance periods of nuclear power plants as well as production levels of both nuclear and conventional power plants in order to meet a power demand, so as to minimize the total production cost. For this application, we used a Dantzig-Wolfe reformulation which allows us to solve realistic instances of the deterministic version of the problem [44]. In practice, the input data comprises a number of uncertain parameters. We deal with a scenario-based stochastic demand with help of a Benders decomposition method. We are working on Multistage Robust Optimization approaches to take into account other uncertain parameters like the duration of each maintenance period, in a dynamic optimization framework. The main challenge addressed in this work is the joint management of different reformulations and solving techniques coming from the deterministic (Dantzig-Wolfe decomposition, due to the large scale nature of the problem), stochastic (Benders decomposition, due to the number of demand scenarios) and robust (reformulations based on duality and/or column and/or row generation due to maintenance extension scenarios) components of the problem [32].

4.4. Resource Allocation for High Performance and Cloud Computing

In the context of numerical simulations on high performance machines, optimizing data locality and resource usage is very important for faster execution times and lower energy consumption. This optimization can be seen as a special case of scheduling problem on parallel resource, with several challenges. First, instances are

typically large: a large matrix factorization (with 50×50 blocks) involves about $30 \cdot 10^3$ tasks. Then, HPC platforms consist of heterogeneous and unrelated resources, what is known to make scheduling problems hard to approximate. Finally, due to co-scheduling effects and shared communication resources, it is not realistic to accurately model the exact duration of tasks. All these observations make it impossible to rely on static optimal solutions, and HPC applications have gone from simple generic static allocations to runtime dynamic scheduling strategies that make their decisions based on the current state of the platform (the location of input data), the expected transfer and running times for the tasks, and some affinity and priority information that have possibly been computed offline. In this context, we are strongly involved in the design of scheduling strategies for the StarPU runtime, with two goals: proving that it is possible to design approximation algorithms whose complexity is extremely small (typically sub-linear in the number of ready tasks), and show that they can be used in practice with good performance results. We are pursuing collaborations both with teams developing the StarPU system (Storm) by designing algorithms for the generic scheduling problems [28], and with teams developing linear algebra algorithms over the runtime (Hiepac), by proposing specialized algorithms for specific cases. For example, in the case of linear algebra applications on heterogeneous platforms, we have considered the combinatorial optimization problem associated to matrix multiplication, that is amenable to partitioning the unit square into zones of prescribed areas while minimizing the overall size of the boundaries. We have improved the best known approximation ratio to 1.15 in [27] and we have shown that the resulting distribution schemes can indeed be used to design efficient implementations using StarPU in [34].

SISTM Project-Team

4. Application Domains

4.1. Systems Biology and Translational medicine

Biological and clinical researches have dramatically changed because of the technological advances, leading to the possibility of measuring much more biological quantities than previously. Clinical research studies can include now traditional measurements such as clinical status, but also thousands of cell populations, peptides, gene expressions for a given patient. This has facilitated the transfer of knowledge from basic to clinical science (from "bench side to bedside") and vice versa, a process often called "Translational medicine". However, the analysis of these large amounts of data needs specific methods, especially when one wants to have a global understanding of the information inherent to complex systems through an "integrative analysis". These systems like the immune system are complex because of many interactions within and between many levels (inside cells, between cells, in different tissues, in various species). This has led to a new field called "Systems biology" rapidly adapted to specific topics such as "Systems Immunology" [45], "Systems vaccinology" [42], "Systems medicine" [34]. From the statistician point of view, two main challenges appear: i) to deal with the massive amount of data ii) to find relevant models capturing observed behaviors.

4.2. The case of HIV immunology

The management of HIV infected patients and the control of the epidemics have been revolutionized by the availability of highly active antiretroviral therapies. Patients treated by these combinations of antiretrovirals have most often undetectable viral loads with an immune reconstitution leading to a survival which is nearly the same to uninfected individuals [38]. Hence, it has been demonstrated that early start of antiretroviral treatments may be good for individual patients as well as for the control of the HIV epidemics (by reducing the transmission from infected people) [33]. However, the implementation of such strategy is difficult especially in developing countries. Some HIV infected individuals do not tolerate antiretroviral regimen or did not reconstitute their immune system. Therefore, vaccine and other immune interventions are required. Many vaccine candidates as well as other immune interventions (IL7, IL15) are currently evaluated. The challenges here are multiple because the effects of these interventions on the immune system are not fully understood, there are no good surrogate markers although the number of measured markers has exponentially increased. Hence, HIV clinical epidemiology has also entered in the era of Big Data because of the very deep evaluation at individual level leading to a huge amount of complex data, repeated over time, even in clinical trials that includes a small number of subjects.

4.3. The case of Ebola vaccine development

In response to the recent outbreak of Ebola virus disease in West Africa, the clinical development of some candidate to Ebola vaccine has been accelerated. Several vectors, mostly encoding glycoprotein of the virus, were tested in Phase I-II studies in order to assess their safety and immunogenicity. One of the main question of interest there is the antibody response induced by vaccination, as some non-human primates studies have shown protection against the virus when antibody levels were high enough. Although bridging studies still have to be developed, antibodies are thus considered as a criterium of interest. The challenge is then to evaluate the durability of the antibody response, whether it be at an individual or population level, in order to evaluate the impact of a vaccine strategy in case of an epidemic. Moreover, we are interested in the factors associated to this antibody response, and even more the other immune markers (from both innate and adaptative immune response) able to predict antibody levels. As those relationship are non-linear, sophisticated statistical and mathematical methods are developed in order to address these questions. A systems medicine approach using multidimensional immunogenicity data from clinical trials and statistical models can help to understand vaccine mechanisms and improve the selection of optimised vaccine strategies for clinical trials.

STORM Project-Team

4. Application Domains

4.1. Application domains benefiting from HPC

The application domains of this research are the following:

- Molecular dynamics (see ExaStamp 7.15),
- Bioinformatics (see ADT Gordon 8.2.2)
- Environment, in particular CO_2 capture (see Exa2PRO, 8.3.1)
- Health and hearth disease analysis (see EXACARD, 8.2.1)
- Software infrastructures for Telecommunications (see AFF3CT, 7.4 , 8.2.2)
- Aéronautique (collaboration avec Airbus, J.-M. Couteyen)

4.2. Application in High performance computing/Big Data

Most of the research of the team has application in the domain of software infrastructure for HPC and BigData (see HPC Cloud Computing project 8.1 , ANR SOLHAR 8.2.1 , Inria ADT SwLoc, Gordon8.2.2 , IPL HAC-SPECIS and BigData 8.2.3 , PIA project ELCI 8.2 , FP7 projects INTERTWinE and Exa2Pro 8.3.1 and PRACE project PRACE5IP 8.3.2).

TADAAM Project-Team

4. Application Domains

4.1. Mesh-based applications

TADAAM targets scientific simulation applications on large-scale systems, as these applications present huge challenges in terms of performance, locality, scalability, parallelism and data management. Many of these HPC applications use meshes as the basic model for their computation. For instance, PDE-based simulations using finite differences, finite volumes, or finite elements methods operate on meshes that describe the geometry and the physical properties of the simulated objects. This is the case for at least two thirds of the applications selected in the 9th PRACE. call ⁰, which concern quantum mechanics, fluid mechanics, climate, material physic, electromagnetism, etc.

Mesh-based applications not only represent the majority of HPC applications running on existing supercomputing systems, yet also feature properties that should be taken into account to achieve scalability and performance on future large-scale systems. These properties are the following:

Size Datasets are large: some meshes comprise hundreds of millions of elements, or even billions.

Dynamicity In many simulations, meshes are refined or coarsened at each time step, so as to account for the evolution of the physical simulation (moving parts, shockwaves, structural changes in the model resulting from collisions between mesh parts, etc.).

Structure Many meshes are unstructured, and require advanced data structures so as to manage irregularity in data storage.

Topology Due to their rooting in the physical world, meshes exhibit interesting topological properties (low dimensionality embedding, small maximum degree, large diameter, etc.). It is very important to take advantage of these properties when laying out mesh data on systems where communication locality matters.

All these features make mesh-based applications a very interesting and challenging use-case for the research we want to carry out in this project. Moreover, we believe that our proposed approach and solutions will contribute to enhance these applications and allow them to achieve the best possible usage of the available resources of future high-end systems.

⁰<http://www.prace-ri.eu/prace-9th-regular-call/>